

Characteristics of Supercritical Transitional Mixing Layers

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The turbulent mixing of fluids at high pressure is a topic of much interest because it is relevant to many combustion applications. Such applications include Diesel engines, gas turbine engines and liquid rockets. Liquid rocket combustion conditions present a particular experimental challenge as the operating regime is supercritical with respect to both fuel and oxidizer and the mixture is potentially explosive. In this situation, numerical simulations with validated models can contribute information that would be otherwise impossible to obtain experimentally.

The modeling of supercritical fluid behavior has been so far primarily addressed in the context of drop modeling, bypassing the turbulent aspect of the flows of practical interest. Among such numerous studies, the investigation of Harstad and Bellan [3] is noteworthy because one of its emphases was the validation of the model; the validation was conducted using the data of Nomura et al. [7]. The model in [3] is based on Keizer's fluctuation-dissipation theory [4] which is totally consistent with non-equilibrium thermodynamics; the resulting

conservation equations contain an enlarged transport matrix including Soret and Dufour effects in the species and energy equations, respectively. This set of equations was mathematically closed with real gas equations of state, and high-pressure transport properties were utilized to obtain corresponding solutions.

Fundamental simulations devoted to supercritical shear flows have not been attempted until very recently (see [6], [8] and [10]). Such fundamental simulations are clearly necessary to unravel the specific aspects of supercritical turbulent shear flows. Examples of specific aspects which have been recently observed by Chehroudi et al. [1], [2], and by Mayer and Tamura [5], include the lack of jet atomization under supercritical condition; instead of drop formation, finger-like structures protruding from the jet are observed.

The present investigation is conducted through Direct Numerical Simulations using the validated set of conservation equations of [3], here in the context of a three-dimensional temporal mixing layer. This mixing layer is perturbed for the purpose of achieving transition and analyze the characteristics of the states thus obtained. The boundary conditions are periodic in the streamwise and spanwise directions, and of outflow type for a real gas (boundary conditions derived by Okong'o et al. [9]) in the streamwise direction. The lower stream contains the higher density fluid, and the initial conditions are supercritical for the species in both streams. The results focus on the examination of the transitional states thus achieved, and on their peculiarities compared to purely gaseous mixing layers. Global features of the mixing layer are assessed for several values of the initial Reynolds number and for several perturbation wavelengths [10]. The examined global quantities, appropriately non-dimensionalized, include the vorticity thickness, the momentum thickness, the momentum thickness based Reynolds number, the positive spanwise vorticity, and the enstrophy. These global features as well as detailed vorticity contour plots show that transition has been attained, but that the transitional state has different characteristics according to the perturbation wavelength. Various features of the mixing layer are documented at the transitional state. Particularly, in contrast to gaseous mixing layers, each simulation displays concentrated regions of very high density gradient magnitude which are convoluted due to

turbulence. In these regions the fluid is primarily the higher density one with small amounts of the lighter fluid dissolved into it. Departures from mixing ideality, indicating the difficulty in mixing at the molecular level (in contrast to ideal mixtures), are identified and are found to increase with increasing density gradient. Strong departures from perfect gas behavior are also displayed by the mixing layer. Moreover, it is shown that even in absence of combustion, the temperature-species PDFs are well correlated (this being attributed to the Soret and Dufour effects), meaning that their joint PDF is not properly approximated by the product of their marginal PDFs. Because under burning conditions the temperature and species will be even more correlated, this indicates that the traditional reactive flow modeling based on replacing the joint PDF representing the reaction rate by the product of the marginal PDFs is not appropriate.

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